Spray Combustion Modeling Including Detailed Chemistry

Eva Gutheil

Interdisziplinäres Zentrum für Wissenschaftliches Rechnen, Universität Heidelberg
Im Neuenheimer Feld 368, 69120 Heidelberg, Germany

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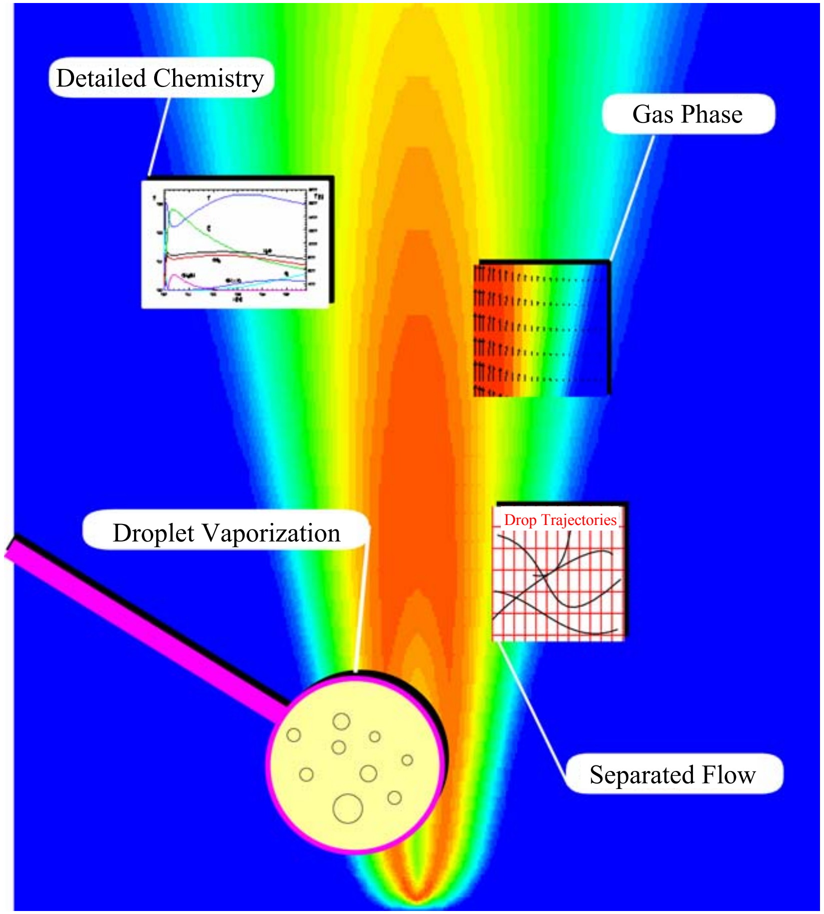
I. Why Detailed Chemisty?

II. Structures of Spray Flames in the Counterflow Configuration

III. Turbulent Spray-Flame Modeling

IV. Summary and Conclusions

Modeling of Technical Spray Flames



Why Detailed Chemistry?

Detailed Chemical Reaction Mechanisms are Available for a Considerate Number of Relevant Combustion Systems (Alcanes, Alcohols, Hydrogen/Air, Hydrogen/Oxygen, …)

- Combustion of liquid fuel sprays in air (e.g. internal engine combustion, industrial furnaces, gas turbine combustors)
- Liquid oxygen in (gaseous) hydrogen (liquid rocket propulsion)
- Liquid oxygen in gaseous hydrocarbons or alcohols (green propellants)

Advantages of Using Detailed Chemistry:

- Mechanism is independent of the experimental configuration, it depends only on pressure (not for hydrogen/air or hydrogen/oxygen)
- Mechanism is the base for development of reduced mechanisms (both manually or automatically developed systems)
- Prediction of pollutants and precursors of soot formation

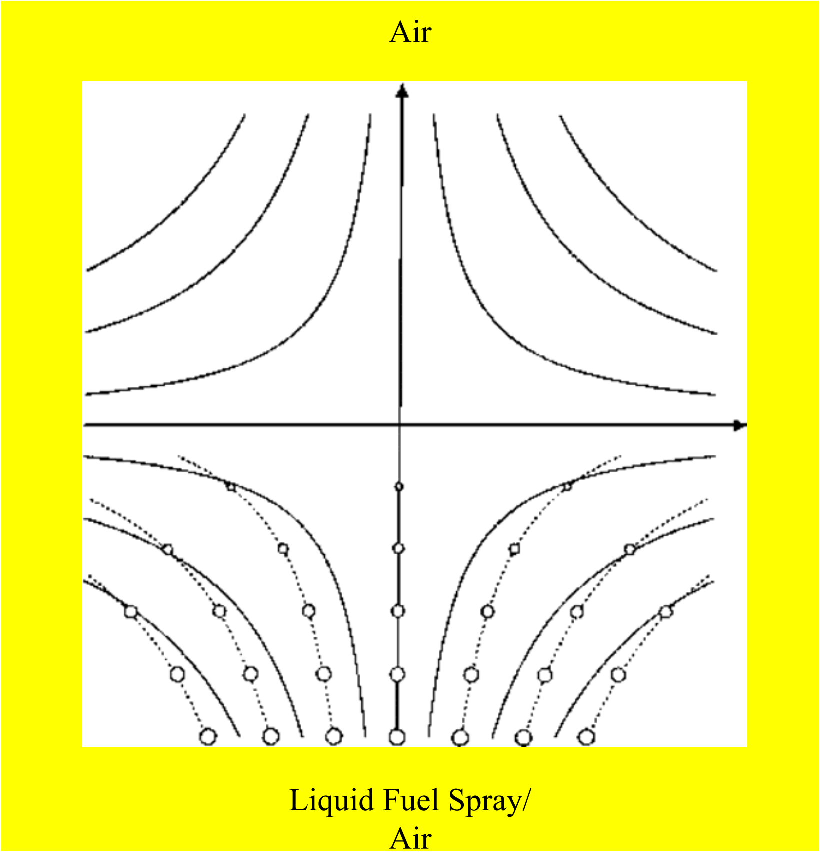
Disadvantages of Using Detailed Chemistry:

- Stiffness of the conservation equations
- Consume a considerable amount of computer time

Applications:

Laminar Flames: Detailed mechanisms can be implemented directly for hydrogen and small hydrocarbons and alcohols
Turbulent Flames: Detailed chemistry may be implemented through use of the flamelet model

Modeling of Laminar Spray Flames
in the Counterflow Configuration



Motivation:

Investigation of laminar spray flame structures using detailed models for instance for chemical reactions

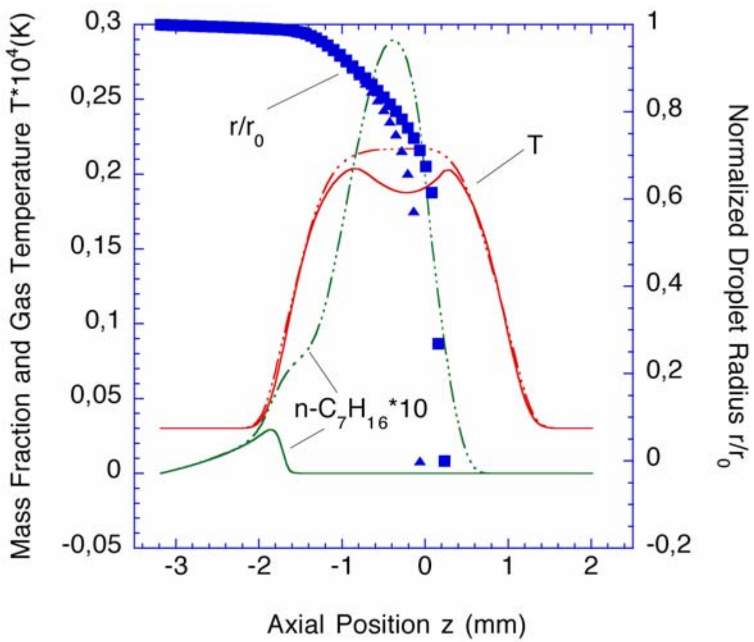
Flamelet modeling of turbulent spray diffusion flames

Properties:

- Planar or axisymmetric
- Two-dimensional
- Strained

Detailed Versus One-Step Chemistry

n-Heptane/Air Spray Flame at Atmospheric Pressure



a = 500/s

Detailed Chemistry:

Solid Lines, Square

One-Step Chemistry:

Dashed Lines, Triangles

$\Rightarrow$ One-Step Chemistry is not Suitable to Correctly Predict Even the Outer Flame Structure

Gutheil, E., Sirignano, W. A.: *Counterflow Spray Combustion Modeling Including Detailed Transport and Detailed Chemistry*, Combustion and Flame: 113(2), 92-105 (1998).

Mathematical Model

Gas-phase with dilute spray

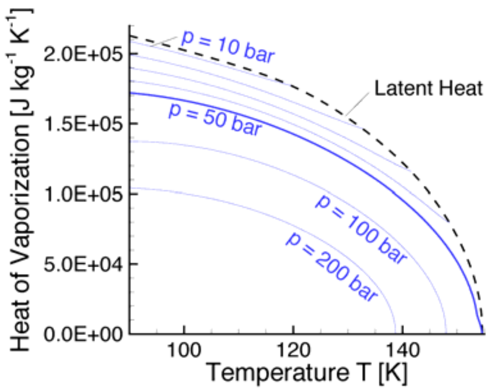
- Boundary layer approximation, low Mach number
- Dimensionless, steady equations
- Similarity transformation $\Rightarrow$ 2D $\rightarrow$ 1D equations
- Ideal gas law
- Detailed chemical reaction mechanisms.
    - **H_2/O_2** (8 species and 38 elementary reactions)
    - **methanol/air** (23 species and 170 elementary reactions)
- Detailed transport: molecular diffusion and thermo diffusion
- Gas-phase properties between 300 and 5000 K from NASA polynomials
- Physical properties of H_2 and O_2 in the range of 80 to 300 K and 1 to 200 bar from *JSME* tables

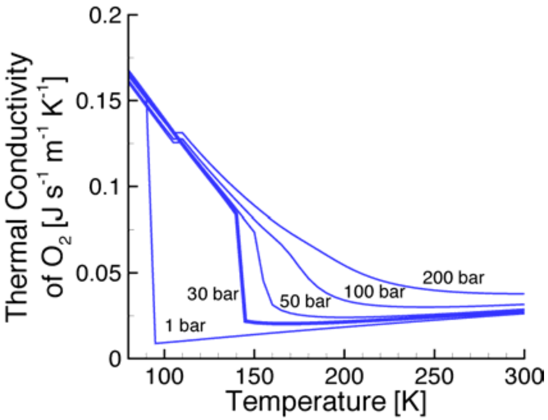
Mathematical Model

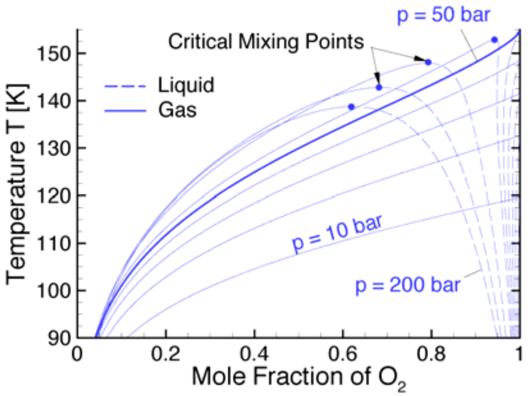
Liquid phase

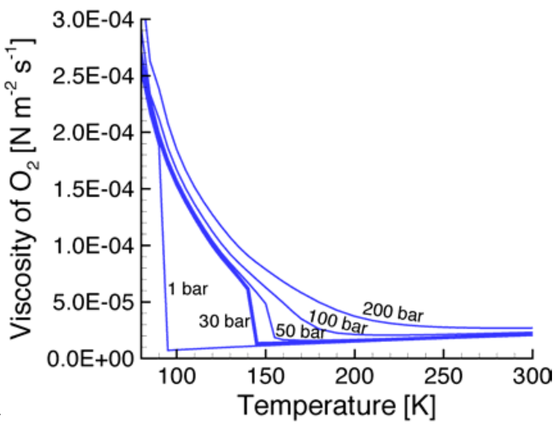
- Mono-, bi- and polydisperse sprays, single-component sprays
- Discrete droplet model
- Spherically symmetric droplets
- Convective droplet model for heating and vaporization (Abramzon-Sirignano model)
- Pressure and temperature dependent heat of vaporization
- Assumption of thermodynamic equilibrium:
  - Ambrose's equation for the evaluation of the vapor pressure for methanol/air
  - Calculation of binary H_2/O_2 mixtures to obtain the gas mixture composition at the interface (replacement of Raoult's law)
- Droplet motion (drag)

Physical Properties of Oxygen (Cryogenic, High Pressure)









Yang, V., Lin, N.N. , Shuen, J.S. , *Combust. Sci. and Tech.*, 97: pp. 247-270, 1994

JSME Data Book, Thermophysical Properties of Fluids, 1983.

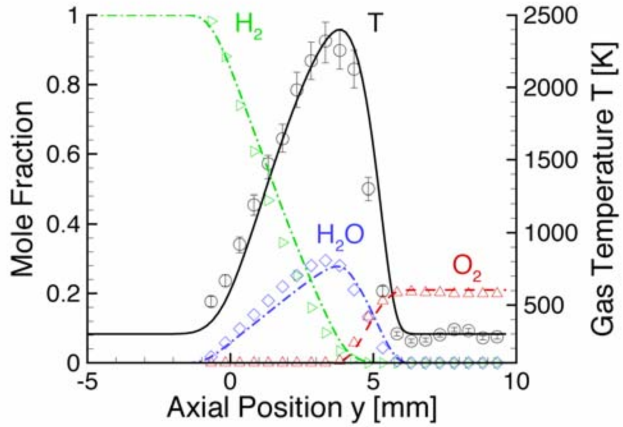
Prausnitz, J.M., Lichtenthaler, R.N., de Avezedo, E.G. , *Molecular Thermo-dynamics of Fluid-Phase Equilibria*, Prentice-Hall, New Jersey, 1986.

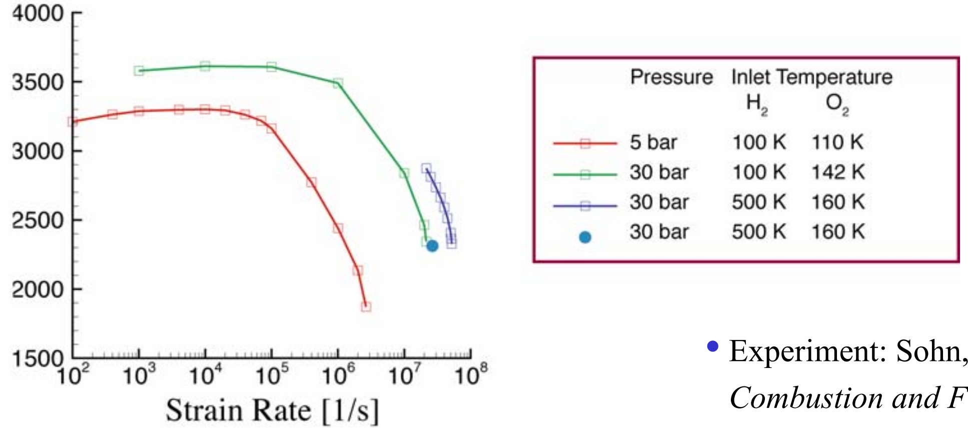
Litchford, R.R., Jeng, S.M., *AIAA Paper* 90-2191, 1990.

H_2/Air Spray Flame at Atmospheric Pressure

$p = 1$ bar, $T_+ = T_- = 300$ K, $a = 100$/s

Symbols: Experiment: T. M. Brown *et. al.*, *Combust. Sci. and Tech.*, Vol. 129, pp. 71-88, 1997.

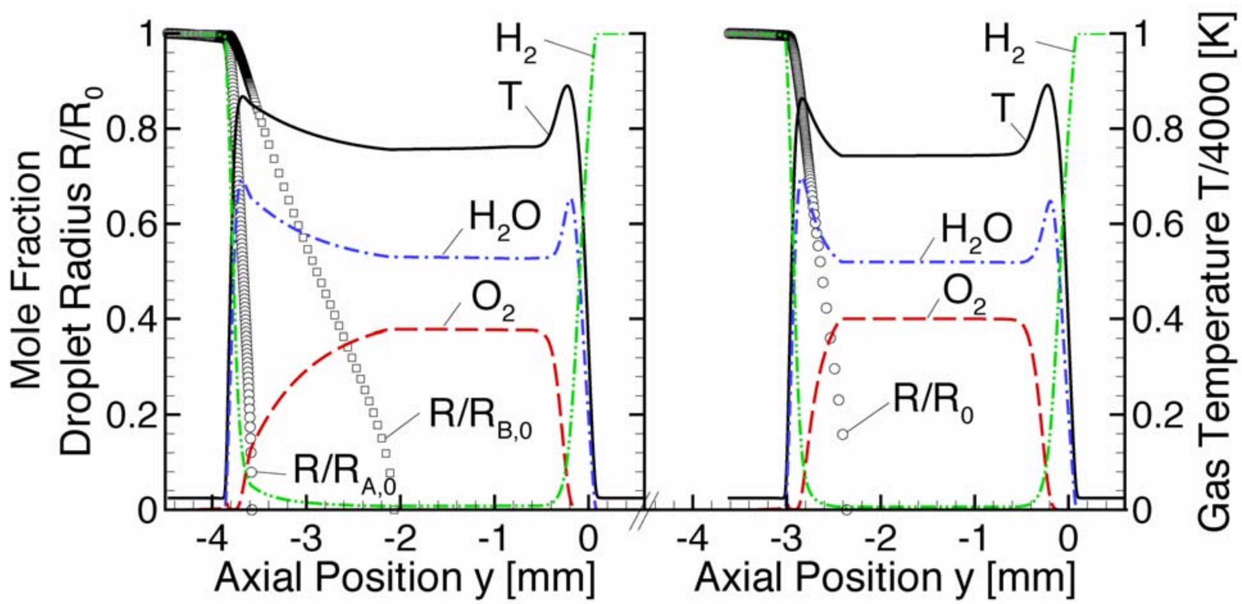




- Experiment: Sohn, C. H., Chung, S. H., Lee, S. R., Kim, J. S., *Combustion and Flame*, 115 (3): 299-312, 1998.

LOX/H_2 Spray Flame

bidisperse **monodisperse**

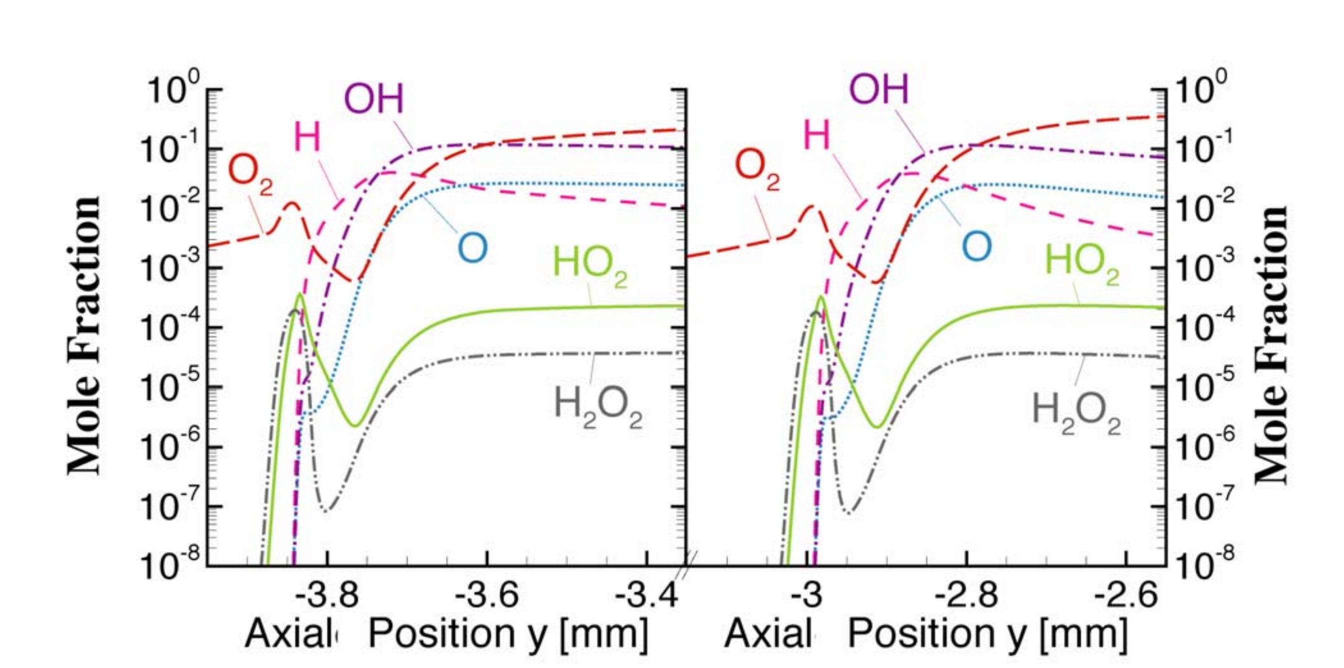


p = 30 bar, Φ = 6, a = 3,000/s (spray side), $R_{A,0}$ = 10 µm, $R_{B,0}$ = 25 µm, SMR_0 = 14.3 µm

Schlotz, D., Gutheil, E.: *Modeling of Laminar Mono- and Bidisperse Liquid Oxygen/Hydrogen Spray Flames in the Counterflow Configuration*, Combustion Science and Technology, 158, 195-210 (2000).

LOX/H_2 Spray Flame

bidisperse **monodisperse**



p = 30 bar, Φ = 6, a = 3,000/s (spray side), $R_{A,0}$ = 10 μm, $R_{B,0}$ = 25 μm, SMR_0 = 14.3 μm

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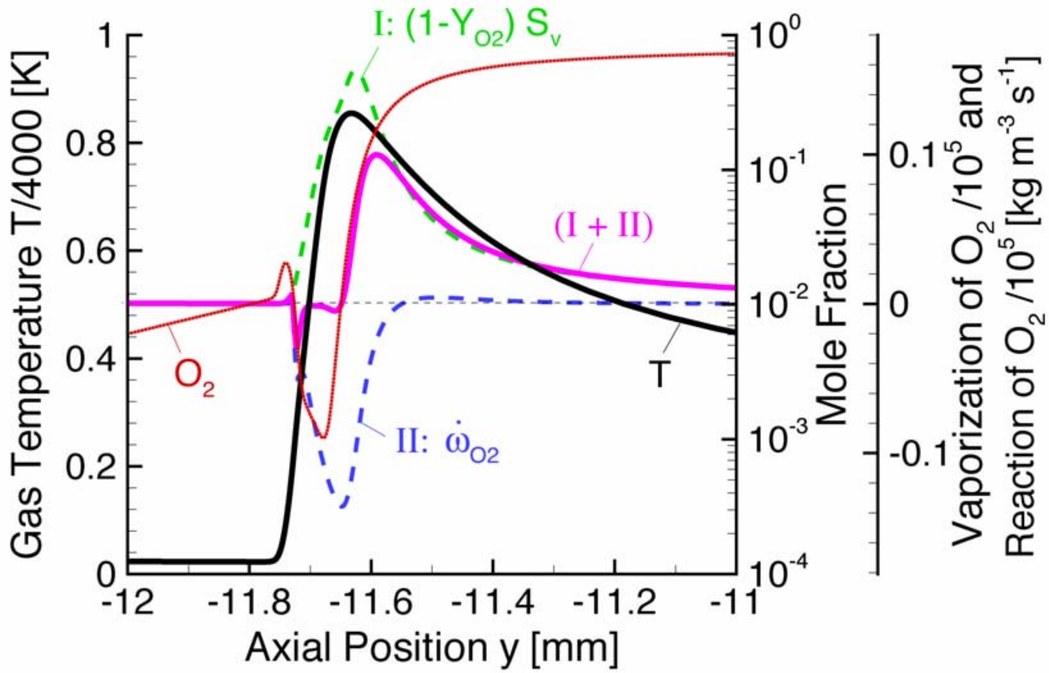
LOX/H_2 Spray Flame

Chemical Reaction Rate and Vaporization Rate



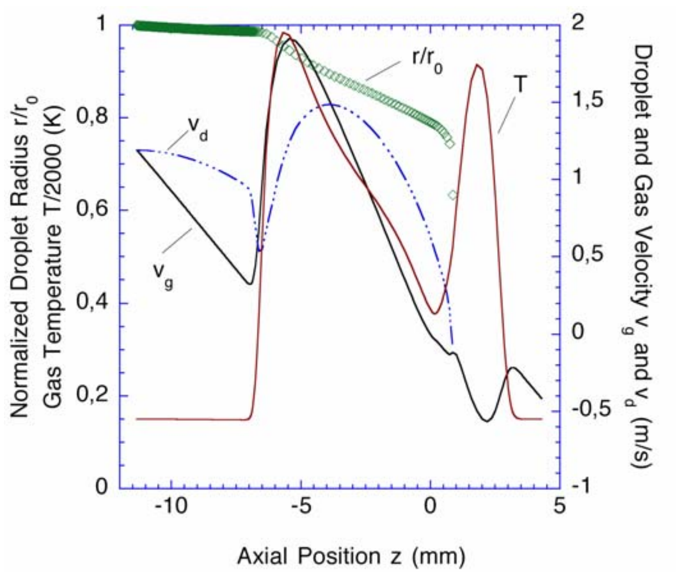
p = 30 bar, Φ = 6, a = 3,000/s (spray side), $R_{A,0}$ = 10 µm, $R_{B,0}$ = 25 µm, SMR_0 = 14.3 µm

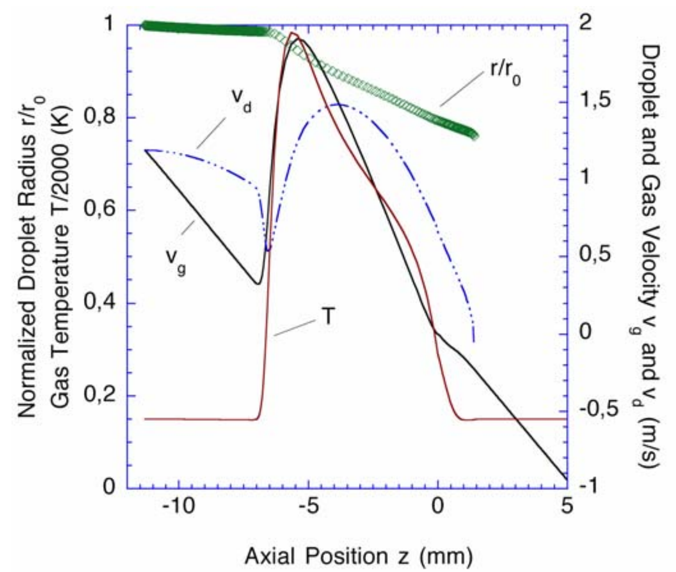
Schlotz, D., Gutheil, E.: *Modeling of Laminar Mono- and Bidisperse Liquid Oxygen/Hydrogen Spray Flames in the Counterflow Configuration*, Combustion Science and Technology, 158, 195-210 (2000).

Multiple Structures of Spray Flames

Methanol/Air Spray Flame at Atmospheric Pressure

***a* = 100/s**



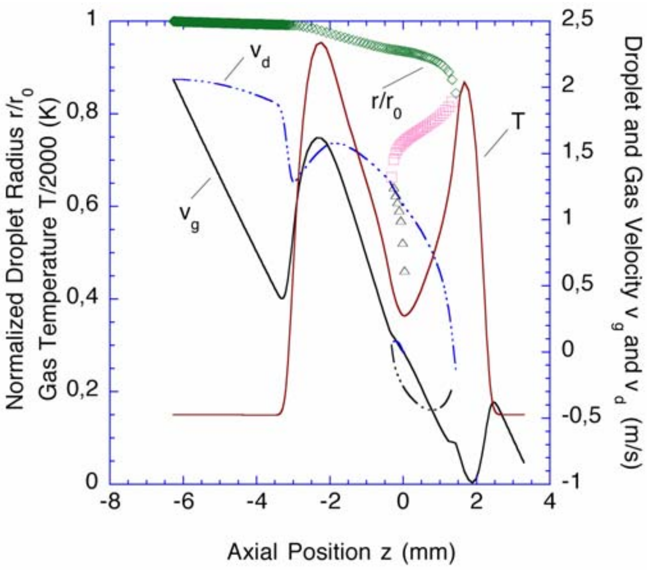


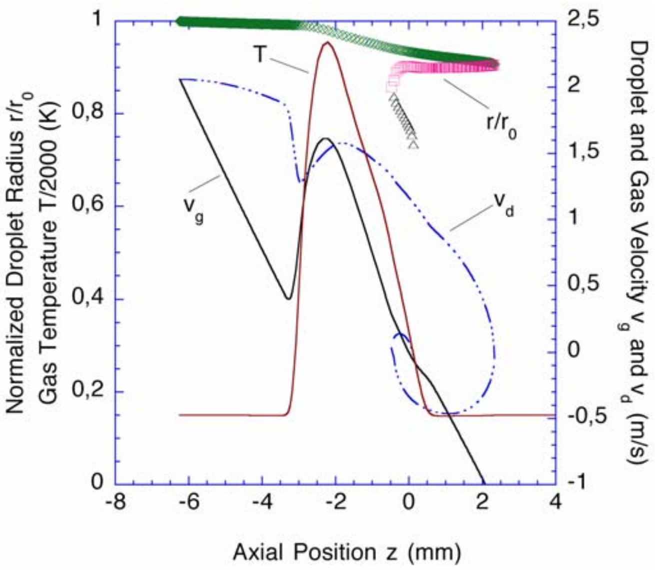
Gutheil, E.: *Multiple Solutions for Structures of Laminar Counterflow Spray Flames*, Progress in Computational Fluid Dynamics, 2004, to appear.

Multiple Structures of Spray Flames

Methanol/Air Spray Flame at Atmospheric Pressure

a = 300/s

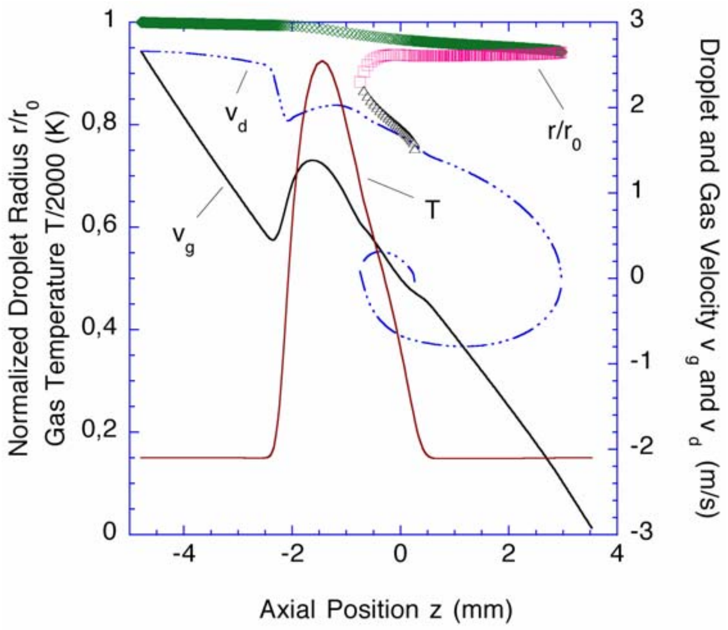




Gutheil, E.: *Multiple Solutions for Structures of Laminar Counterflow Spray Flames*, Progress in Computational Fluid Dynamics, 2004, to appear.

Methanol/Air Spray Flame at Atmospheric Pressure

a= 500/s



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Multiple Structures of Spray Flames

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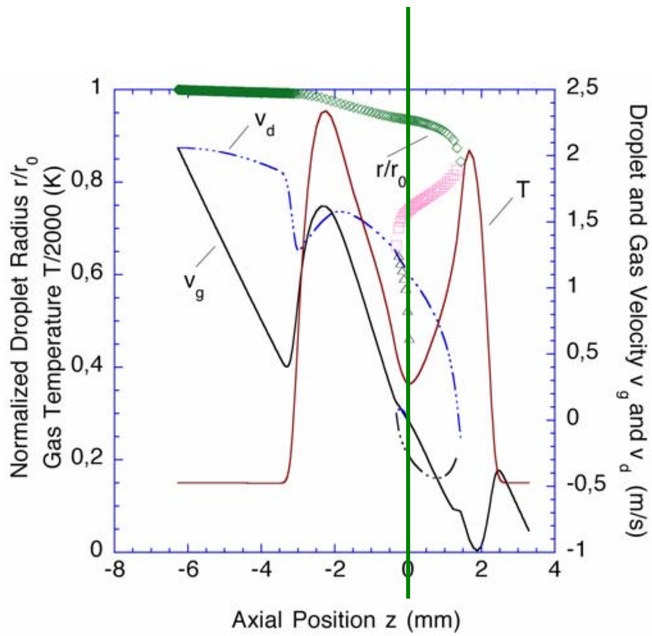
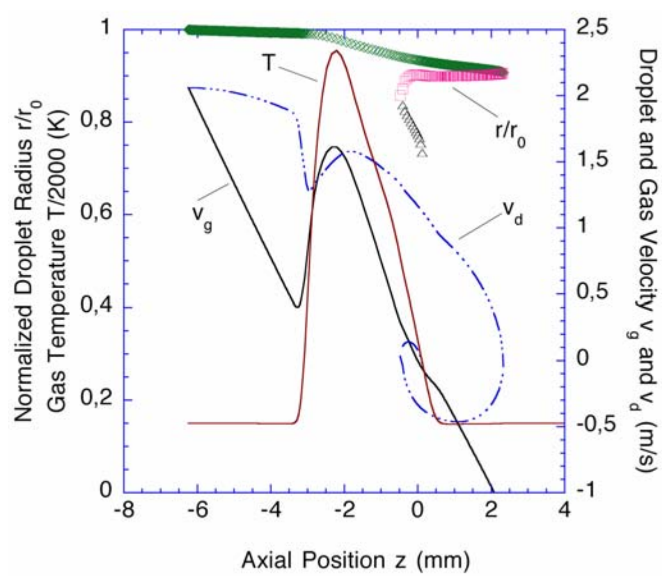




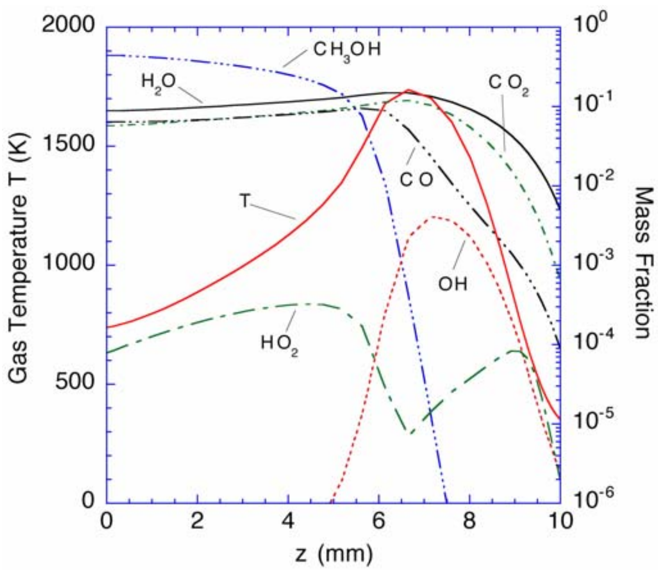
Gutheil, E.: *Multiple Solutions for Structures of Laminar Counterflow Spray Flames*, Progress in Computational Fluid Dynamics, 2004, to appear.

Comparison: Gas-Sided Flame and Pure Gas Flames

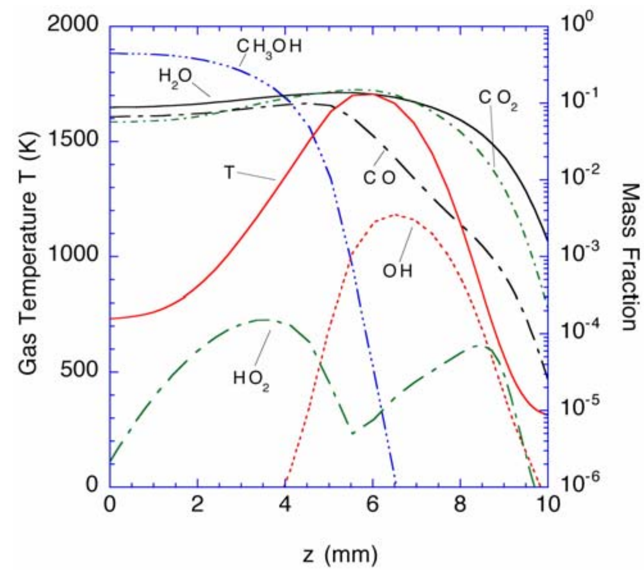
Methanol/Air Spray Flame at Atmospheric Pressure

***a* = 300/s**

Gas Side (Spray Flame)



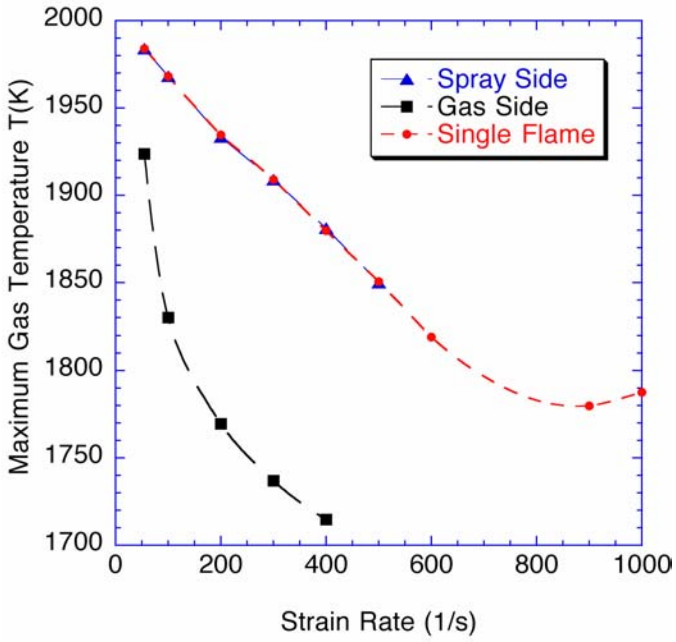
Gas Flame



Gutheil, E.: *Multiple Solutions for Structures of Laminar Counterflow Spray Flames*, Progress in Computational Fluid Dynamics, 2004, to appear.

Methanol/Air Spray Flame at Atmospheric Pressure

Comparison of Spray and Gas Flame



Gutheil, E.: *Multiple Solutions for Structures of Laminar Counterflow Spray Flames*, Progress in Computational Fluid Dynamics, 2004, to appear.

Structures of Laminar Spray Flames in the Counterflow Configuration

- The LOX/H_2 Spray Flames are very stable and persist to strain rates of 25,000/s. The non-monotonicity of the gaseous oxygen profile on the spray side stems from the competition of vaporization and combustion.

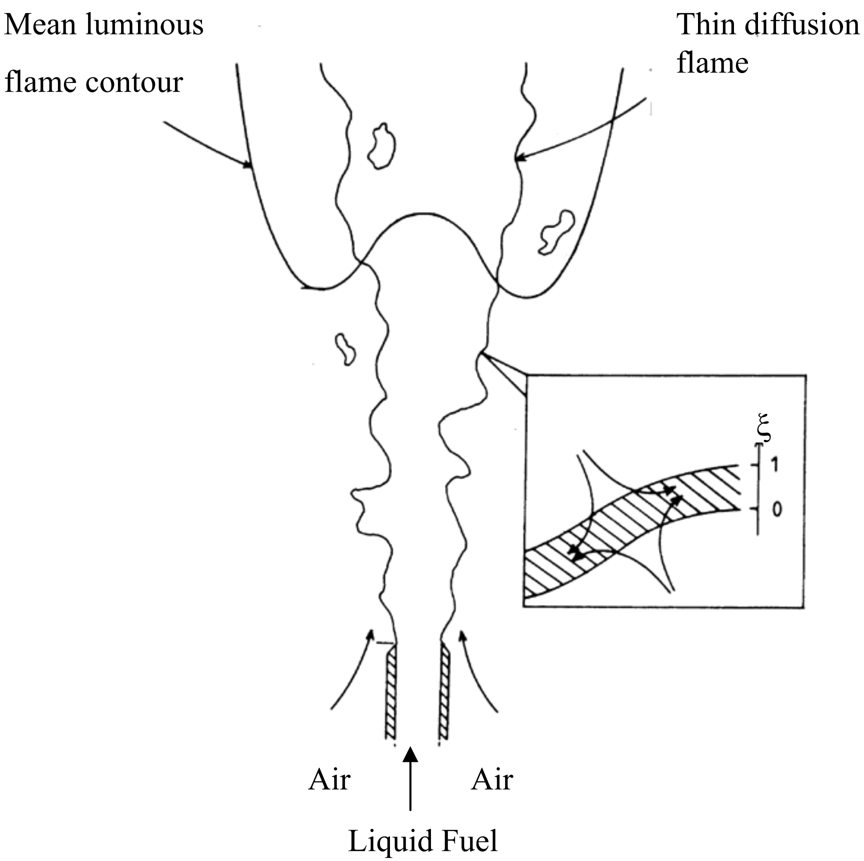
- Multiple structures of methanol/air spray flames have been found for strain rates up to 400/s. The inner structure of the gas-sided flame is the same as a pure gas flamelet with appropriate initial conditions.

- At high strain, the gas-sided flame is extinguished and the spray-sided flame moves towards the gas-side of the counterflow configuration.

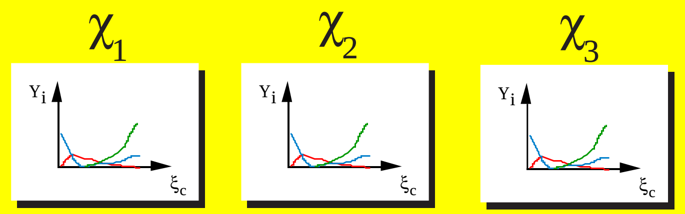
Question: How does the finding affect models such as the flamelet model for turbulent spray diffusion flames?

Flamelet-Model for Turbulent Diffusion Flames

Turbulent Flame



Library of laminar flame structures
in the counterflow configuration

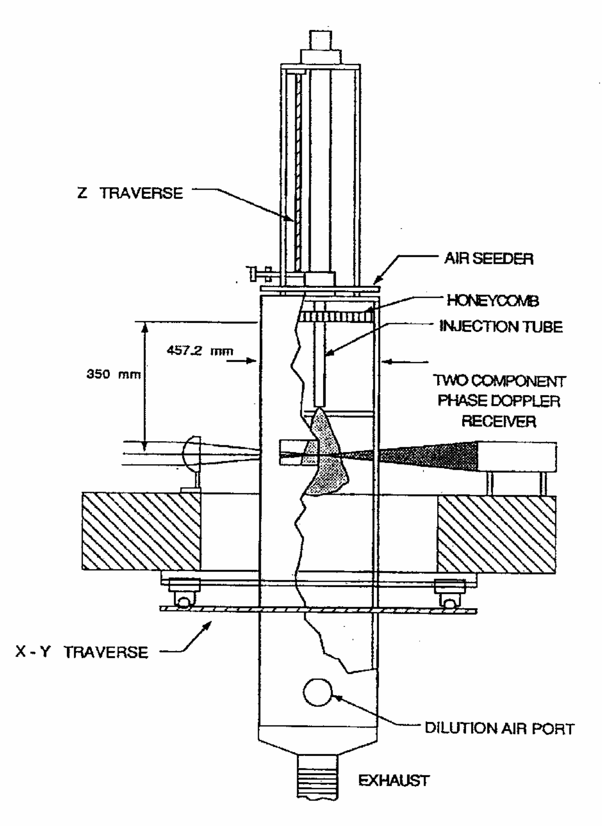


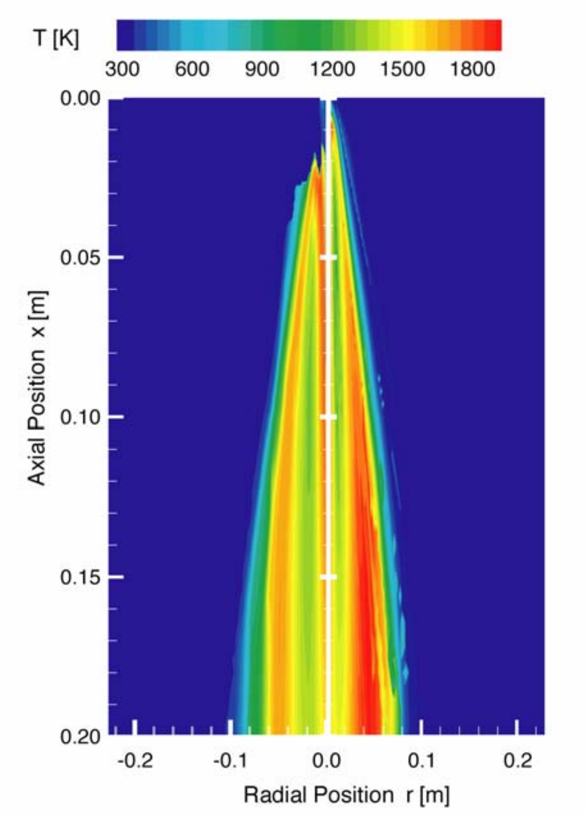
$$\Phi_i = \Phi_i(\xi, \chi)$$

$$\tilde{\Phi}_i = \int_0^\infty \int_0^1 \Phi_i(\xi, \chi)\, \tilde{P}(\xi)\, \tilde{P}(\chi)\, d\xi\, d\chi$$

- Gas flames
  - Strain rate
- Spray flames
  - Strain rate
  - Droplet size
  - Droplet velocity
  - Equivalence ratio

Laminar Spray Flame Structures for Use in Flamelet Models for Turbulent Spray Diffusion Flames (Methanol/Air)





LHS: Gas Flamelets

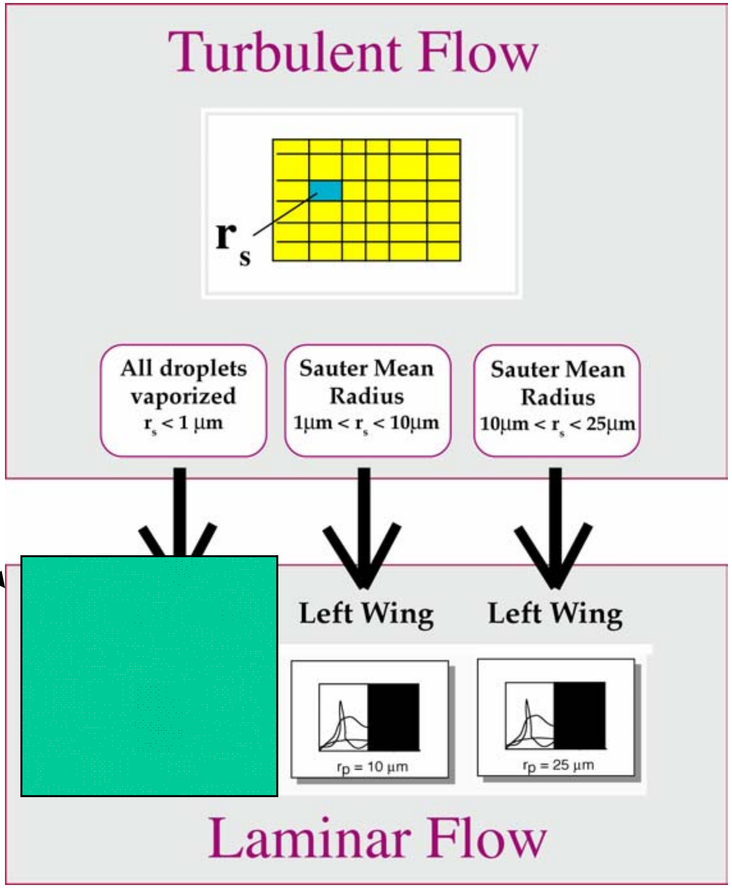
RHS: Spray Flamelets

Experiment: McDonell V.G., Samuelsen, G.S., *UCI-Laboratory Report* UCI-ARTR-90-17A-C (1990)

Simulation: Hollmann, C., Gutheil. E., *Combust. Sci. and Tech*. **135** 1-6, 175 (1998).

Modeling of Turbulent Spray Flames

Replace by Pure Gas Flamelet

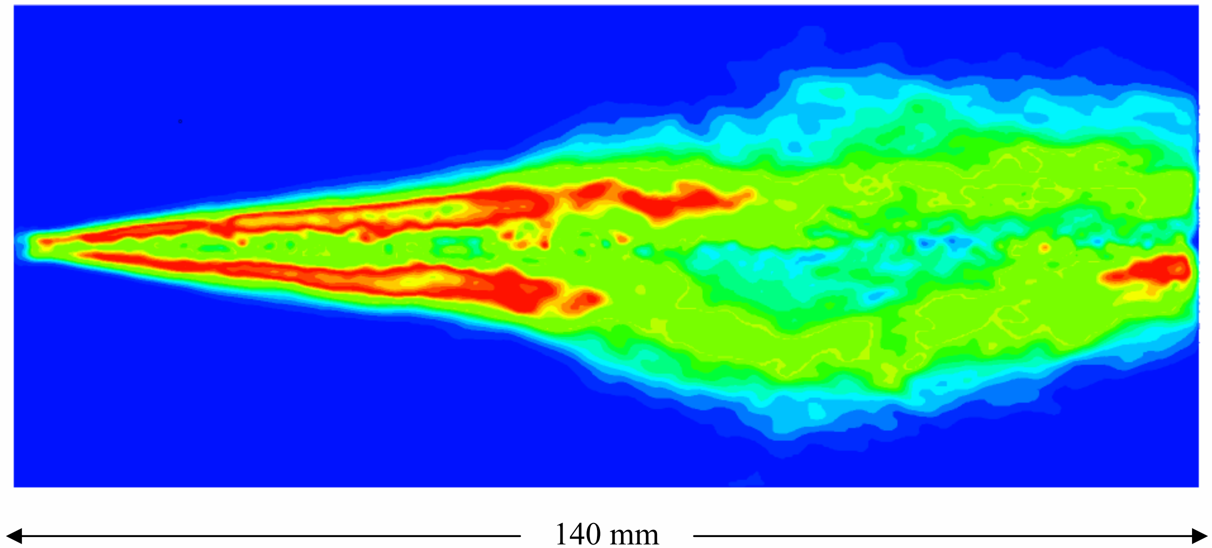


Leads to Simplification of Implementing Laminar Spray Flamelets

Modeling of Turbulent LOX/H_2 Spray Flames

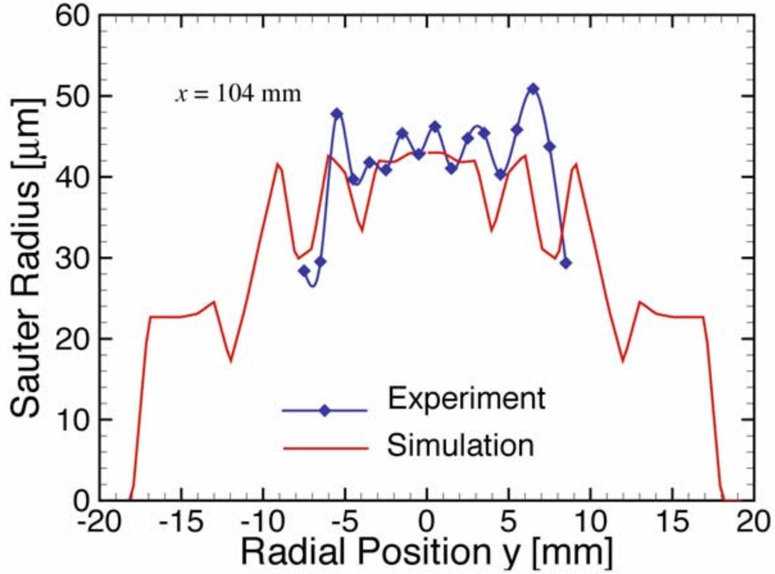
Micro Combustion Chamber M3 (DLR Lampoldshausen)

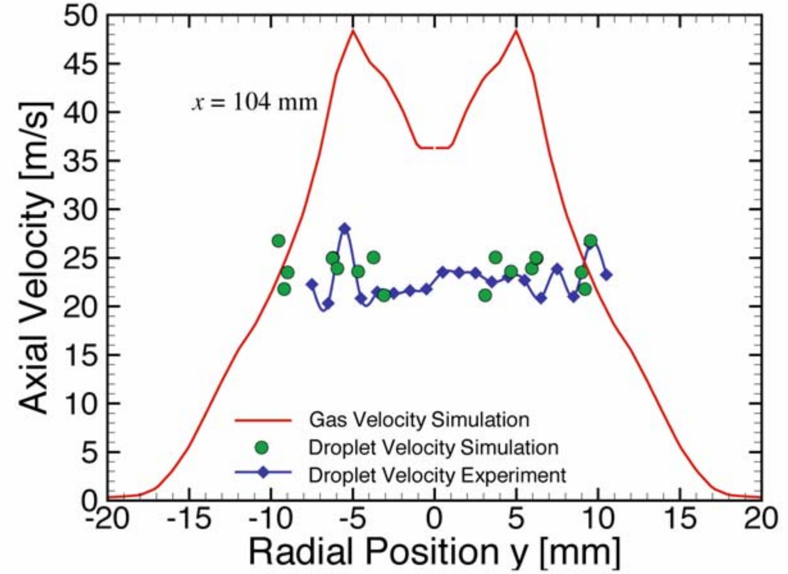
OH-Emission, p = 5 bar, T_0 = 100 K



Sender, J., *et al.*, *Proceedings of the 13th Annual Conference on Liquid Atomization on Spray Systems*, Florence, Italy, 145-154 (1997).

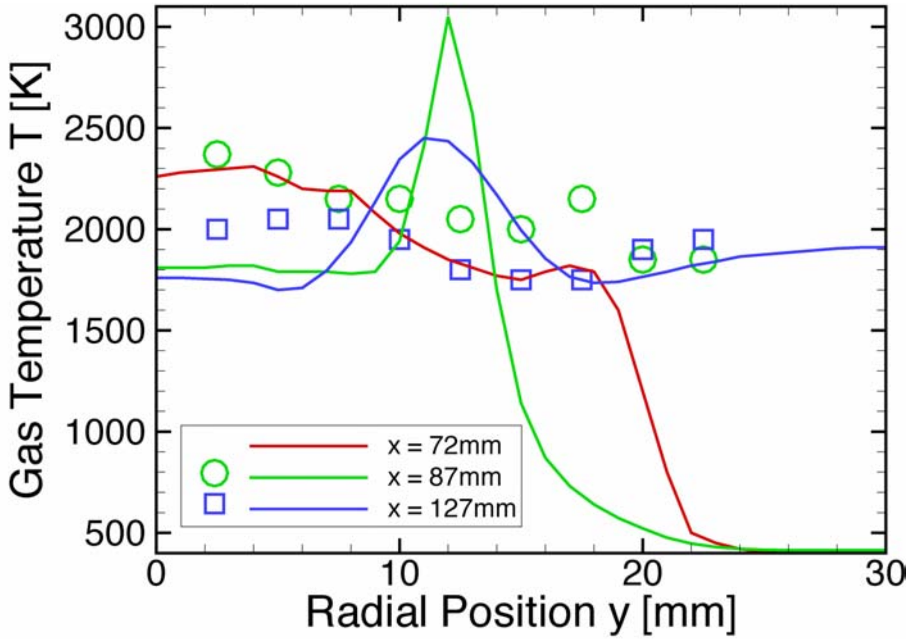
Modeling of Turbulent Spray Flames





Experiment: Sender, J., *et al.*, *Proceedings of the 13th Annual Conference on Liquid Atomization on Spray Systems*, Florence, Italy, 145-154 (1997).
Simulation: Schlotz, D., Brunner, M., Gutheil, E.: *Modeling of Turbulent LOX/*H_2 *Combustion under Cryogenic and Elevated Pressure Conditions*, ILASS Europe Conference, Zürich, September 2-6 (2001).

Modeling of Turbulent Spray Flames



Experiment: Sender, J., *et al.*, *Proceedings of the 13th Annual Conference on Liquid Atomization on Spray Systems*, Florence, Italy, 145-154 (1997).

Simulation: Schlotz, D., Brunner, M., Gutheil, E.: *Modeling of Turbulent LOX/H_2 Combustion under Cryogenic and Elevated Pressure Conditions*, ILASS Europe Conference, Zürich, September 2-6 (2001).

Mixing in Turbulent Sprays

- The β-function that is typically used to describe the mixing in turbulent diffusion flames does not perform well in regions where vaporization is present[1].
- **Here**: Modification of the description of the β-function through use of a transport equation for the probability density function of the mixture fraction, $\tilde{f}$, in turbulent sprays[2]:

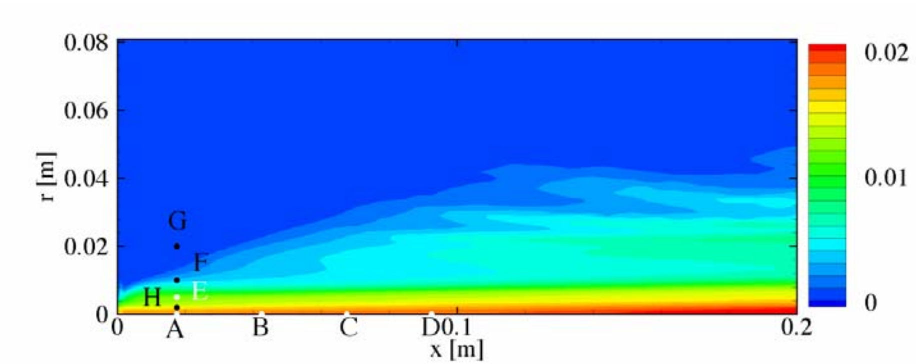
$$\bar{\rho}_g \frac{\partial \tilde{f}}{\partial t} + \bar{\rho}_g U_j \frac{\partial \tilde{f}}{\partial x_j} + \frac{\partial (\bar{\rho}_g \bar{S}_s \tilde{f})}{\partial \zeta_c} = -\frac{\partial}{\partial \zeta_c}\left[\bar{\rho}_g \left\langle \frac{\partial}{\partial x_j}\left(D_M \frac{\partial \xi_c}{\partial x_j} \right) \middle| \zeta_c \right\rangle \tilde{f} \right].$$

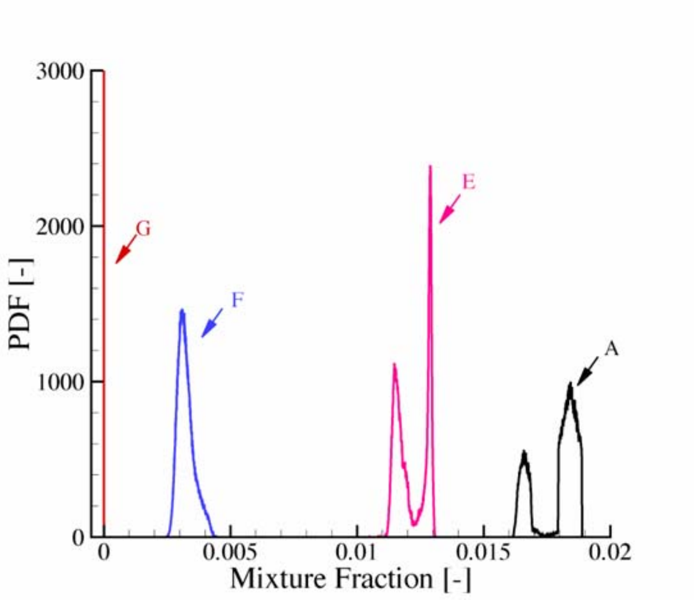
[1]Miller R.S. Bellan, J. On the Validity of the Assumed Probability Density Function Method for Modeling Binary Mixing/ Reaction of Evaporated Vapor in Gas/Liquid-Droplet Turbulent Shear Flow, *Proc. Combust. Inst.* **27**: 1065-1072, 1998.

[2]Ge, H.-W., Gutheil, E.: PDF Simulation of Turbulent Spray Flows, *Atomiz. Sprays*, 2004, submitted.

Mixing in Turbulent Methanol/Air Sprays

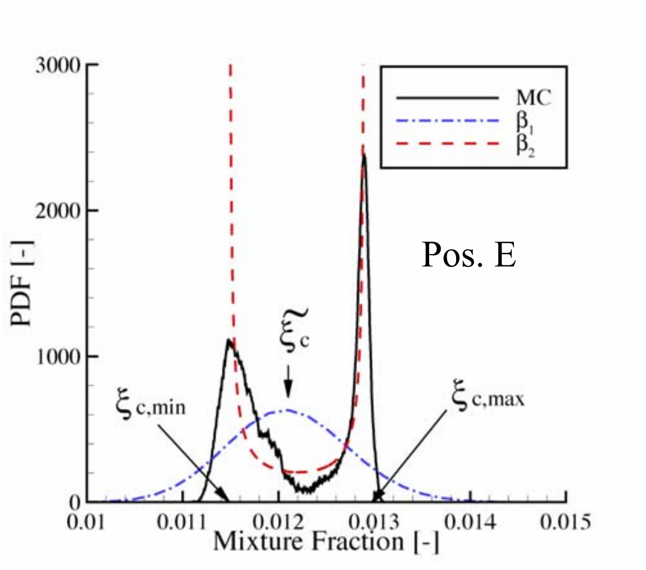
Methanol Vapor Fraction and PDF of the Mixture Fraction

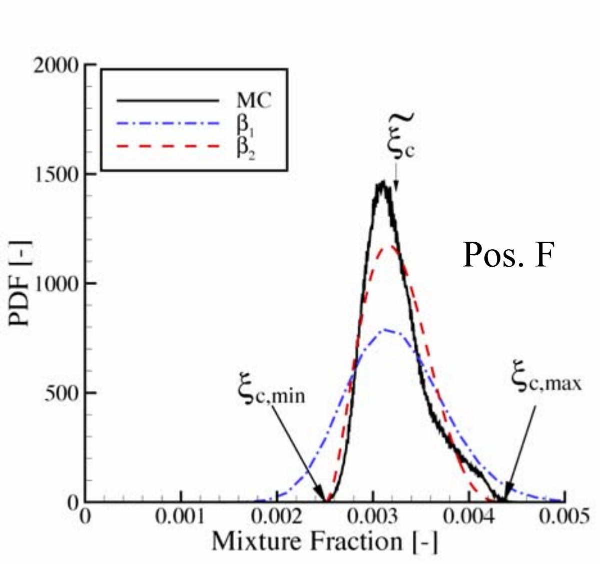




Ge, H.-W., Gutheil, E.: PDF Simulation of Turbulent Spray Flows, *Atomiz. Sprays*, 2004, submitted.

Probability Density Functions at Various Positions





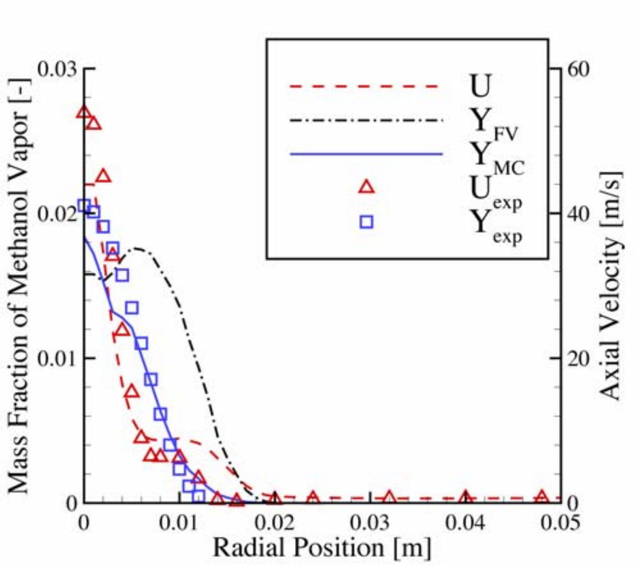
$$P(\xi_c) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \xi_c^{\alpha-1} (1-\xi_c)^{\beta-1}$$

$$P(\xi_c) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} (\xi_{c,\max} - \xi_{c,\min})^{1-\alpha-\beta} (\xi_c - \xi_{c,\min})^{\alpha-1} (\xi_{c,\max} - \xi_c)^{\beta-1}$$

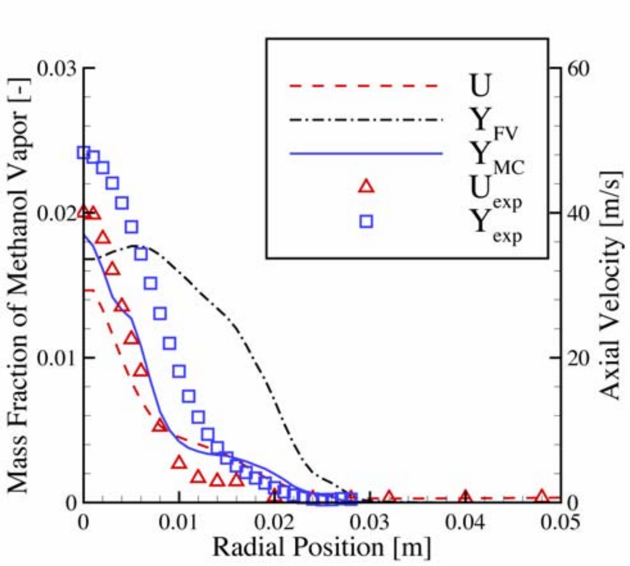
Ge, H.-W., Gutheil, E.: PDF Simulation of Turbulent Spray Flows, *Atomiz. Sprays*, 2004, submitted.

Comparison of Results with Presumed and Monte-Carlo PDF, and with Experiment

x = 25 mm



x = 50 mm



Experiment: McDonell, V. G. and Samuelsen, G.S., An Experimental Data Base for Computational Fluid Dynamics of Reacting and Nonreacting Methanol Sprays, *J. Fluids Engin.* **117**: 145-153, 1995.

Simulation: Ge, H.-W., Gutheil, E.: PDF Simulation of Turbulent Spray Flows, *Atomiz. Sprays*, 2004, submitted.

Summary and Conclusions

- LOX/H_2 spray flames in the counter-flow configuration have been studied, and the gaseous oxygen profile shows a non-monotonic behavior because of the high reactivity of the system. The flames persist to strain rates up to 25,000/s, and extinction has not yet been found.

- Multiple structures of laminar methanol/air counter-flowing spray flames have been identified at low strain rates up to 400/s on the spray side of the configuration for the present conditions. The gas-sided spray flame shows the same inner structure as a pure gas flamelet with appropriate boundary conditions, and this simplifies the implementation of the flamelet model for turbulent spray diffusion flames.

- The assumed β-function for the turbulent mixing in spray flames is poor in regions where vaporization exists, and it has been replaced by a PDF transport equation for the mixture fraction. A modified β-function is suitable to predict the shape of the PDF of the mixture fraction.

Future Research

- Extension of the model to unsteady flamelets
- Application of the PDF method to turbulent spray flame simulations
- Extension to other liquids